

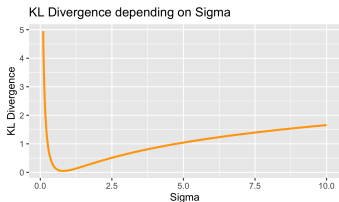
Introduction to Machine Learning

Kullback-Leibler Divergence



Learning goals

- Know the KL divergence as distance between distributions
- Understand KL as expected log-difference
- Understand how KL can be used as loss
- Understand that KL is equivalent to the expected likelihood ratio



KULLBACK-LEIBLER DIVERGENCE

We now want to establish a measure of distance between (discrete or continuous) distributions with the same support for $X \sim p(X)$:

$$D_{KL}(p||q) = \mathbb{E}_{X \sim p} \left[\log \frac{p(X)}{q(X)} \right] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)},$$

or:

$$D_{KL}(p||q) = \mathbb{E}_{X \sim p} \left[\log \frac{p(X)}{q(X)} \right] = \int_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx.$$

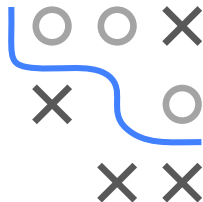
In the above definition, we use the conventions that $0 \log(0/0) = 0$, $0 \log(0/q) = 0$ and $p \log(p/0) = \infty$ (based on continuity arguments where $p \rightarrow 0$). Thus, if there is any realization $x \in \mathcal{X}$ such that $p(x) > 0$ and $q(x) = 0$, then $D_{KL}(p||q) = \infty$.



KULLBACK-LEIBLER DIVERGENCE / 2

$$D_{KL}(p||q) = \mathbb{E}_{X \sim p} \left[\log \frac{p(X)}{q(X)} \right]$$

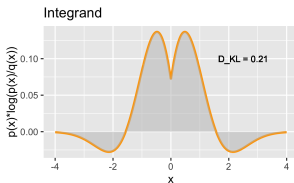
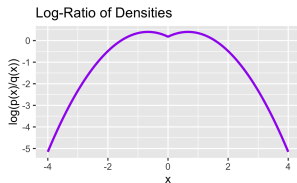
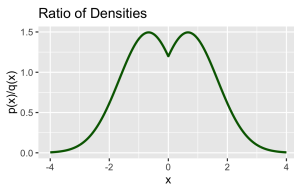
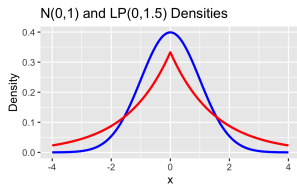
- What is the intuition behind this formula?
- We will soon see that KL has quite some value in measuring “differences” but is not a true distance.
- We already see that the formula is not symmetric and it often makes sense to think of p as the first or original form of the data, and q as something that we want to measure the quality of with reference to p .



KL-DIVERGENCE EXAMPLE

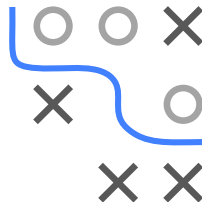
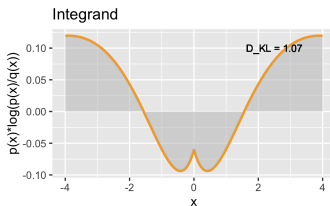
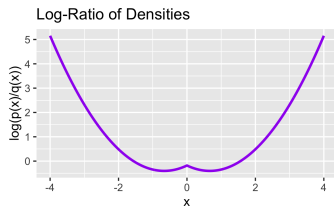
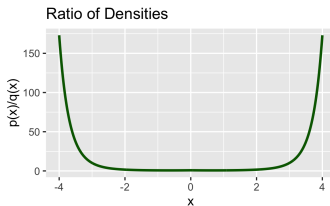
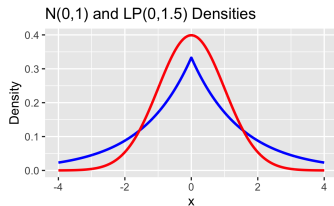
KL divergence between $p(x) = N(0, 1)$ and $q(x) = LP(0, 1.5)$ given by

$$D_{KL}(p||q) = \int_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)}.$$



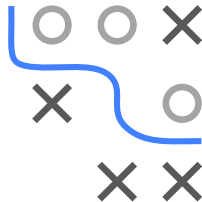
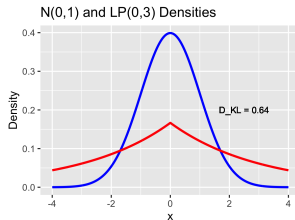
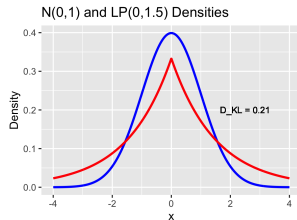
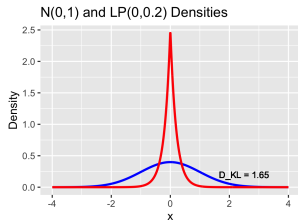
KL-DIVERGENCE EXAMPLE

KL divergence between $p(x) = LP(0, 1.5)$ and $q(x) = N(0, 1)$ is different since KL not symmetric



KL-DIVERGENCE EXAMPLE

KL divergence of $p(x) = N(0, 1)$ and $q(x) = LP(0, \sigma)$ for varying σ



INFORMATION INEQUALITY

$D_{KL}(p||q) \geq 0$ holds always true for any pair of distributions, and holds with equality if and only if $p = q$.

We use Jensen's inequality. Let A be the support of p :

$$\begin{aligned} -D_{KL}(p||q) &= -\sum_{x \in A} p(x) \log \frac{p(x)}{q(x)} \\ &= \sum_{x \in A} p(x) \log \frac{q(x)}{p(x)} \\ &\leq \log \sum_{x \in A} p(x) \frac{q(x)}{p(x)} \\ &\leq \log \sum_{x \in \mathcal{X}} q(x) = \log(1) = 0 \end{aligned}$$

As \log is strictly concave, Jensen also tells us that equality can only happen if $q(x)/p(x)$ is constant everywhere. That implies $p = q$.



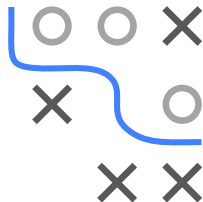
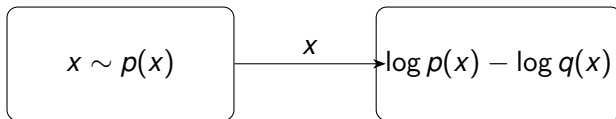
KL AS LOG-DIFFERENCE

Suppose that data is being generated from an unknown distribution $p(x)$ and we model $p(x)$ using an approximating distribution $q(x)$.

First, we could simply see KL as the expected log-difference between $p(x)$ and $q(x)$:

$$D_{KL}(p||q) = \mathbb{E}_{x \sim p}[\log(p(x)) - \log(q(x))].$$

This is why we integrate out with respect to the data distribution p . A “good” approximation $q(x)$ should minimize the difference to $p(x)$.



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The figure consists of four subplots arranged in a 2x2 grid, illustrating the relationship between a Normal distribution $N(0, 1)$ and a Laplace distribution $LP(0, 3)$.

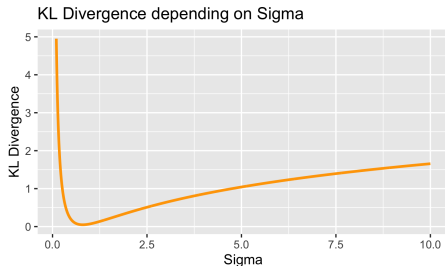
- Top Left:** Plot of **Density** versus **x**. The x-axis ranges from -4 to 4, and the y-axis ranges from 0.0 to 0.4. The blue curve represents the $N(0, 1)$ density, which is a standard normal distribution centered at 0. The red curve represents the $LP(0, 3)$ density, which is a Laplace distribution centered at 0 with a scale parameter of 3. The two curves intersect at approximately $x = \pm 1.5$.
- Top Right:** Plot of **Log-Density** versus **x**. The x-axis ranges from -4 to 4, and the y-axis ranges from -7.5 to -2.5. The blue curve represents $\log(p(x))$ and the red curve represents $\log(q(x))$. The area between the two curves is shaded gray, representing the log-likelihood ratio.
- Bottom Left:** Plot of **Expectation Difference** versus **x**. The x-axis ranges from -4 to 4, and the y-axis ranges from -0.6 to 0.0. The blue curve represents $E[\log(p(x))]$ and the red curve represents $E[\log(q(x))]$. The area between the two curves is shaded gray. The text $D_{KL} = 0.64$ is displayed in the plot.
- Bottom Right:** Plot of **Expectation Ratio** versus **x**. The x-axis ranges from -4 to 4, and the y-axis ranges from 0.0 to 0.3. The orange curve represents $E[\log(p(x)/q(x))]$. The area under the curve is shaded gray. The text $D_{KL} = 0.64$ is displayed in the plot.

KL IN FITTING

In machine learning, KL divergence is commonly used to quantify how different one distribution is from another.

Because KL quantifies the difference between distributions, it can be used as a loss function between distributions.

In our example, we investigated the KL between $p = N(0, 1)$ and $q = LP(0, \sigma)$. Now, we identify an optimal σ which minimizes the KL.



KL AS LIKELIHOOD RATIO

- Let us assume we have some data and want to figure out whether $p(x)$ or $q(x)$ matches it better.
- How do we usually do that in stats? Likelihood ratio!

$$LR = \prod_i \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} \quad LLR = \sum_i \log \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})}$$

If for $\mathbf{x}^{(i)}$ we have $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)}) > 1$, then p seems better, for $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)}) < 1$ q seems better.

- Now assume that the data is generated by p . Can also ask:
- "How to quantify how much better does p fit than q , on average?"

$$\mathbb{E}_p \left[\log \frac{p(X)}{q(X)} \right]$$

That expected LLR is really KL!

